研究成果展開事業
産学共創基礎基盤研究 プログラム

国立研究開発法人 科学技術振興機構

「革新的構造用金属材料創製を目指したヘテロ構造制御に基づく新指導原理の構築」

ハミルトニアンからの材料強度設計
ハミルトニアンからの合金降伏強度予測 - マルチスケールアプローチ

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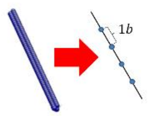
研究・成果概要

Kinetic Monte Carlo model of dislocation motion in dilute iron-based alloy

Shuhei Shinzato, Masato Wakeda, Shigenobu Ogata, "An atomistically informed kinetic Monte Carlo model for predicting solid solution strengthening of body-centered cubic alloys", International Journal of Plasticity, 122, (2019), 319-337.

Atomistic model to coarse grained kMC model

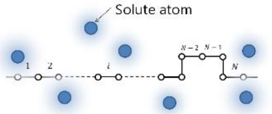
Screw dislocation described as line segments



Each segments have length of unit Burgers vector

Dislocation segment moves on $(\bar{1}10)$ slip plane along $[11\bar{2}]$ direction

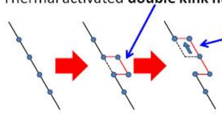
Dislocation moves in solute distributed field



Algorithm of kMC simulation

- Construct the event list
- Calculate the total rate of event list
- Select the event from possible event list
- Execute the selected event
- Update the time with $\delta t = 1/R$
- Update event list

Possible kMC events :
Thermal activated **double kink nucleation** and **kink migration**



Thermal activated kink migration is possible when solutes affect kink migration process

Event rate for forward(+) / backward(-) dislocation motion

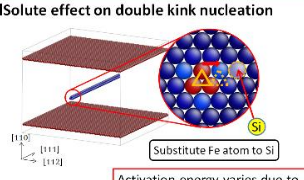
$$R_{\mathrm{kn}}^{+/-} = \nu_{\mathrm{kn}}^{0} \exp\left(-\frac{\Delta G_{\mathrm{kn}}^{+/-}(\tau)}{k_{\mathrm{B}}T}\right) \quad R_{\mathrm{km}}^{+/-} = \nu_{\mathrm{km}}^{0} \exp\left(-\frac{\Delta G_{\mathrm{km}}^{+/-}(\tau)}{k_{\mathrm{B}}T}\right)$$

Time evolution of dislocation with timestep δt

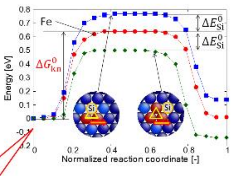
$$t_{n+1} = t_n + \delta t, \quad \delta t = \frac{1}{R} = \left[\sum_{i}^{N_{\mathrm{seg}}} \left(R_{\mathrm{kn},i}^{+/-} + R_{\mathrm{km},i}^{+/-}\right)\right]^{-1}$$

Activation energy on dislocation motion

□**Solute effect on double kink nucleation**

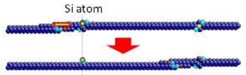


Activation energy varies due to attractive interaction between dislocation and solute Si

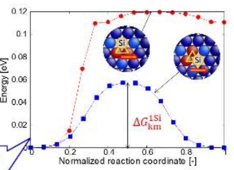


□ **Solute effect on kink migration process**

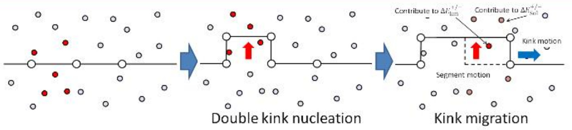
Estimate an activation energy required to overcome Si atom



Kink migration process is affected by both dislocation-solute and direct kink-solute interaction



Modeling of solute-dislocation interaction

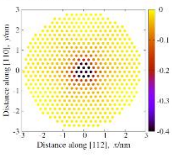


Solute effect: change in total interaction energy on each state

$$\Delta E_{\mathrm{Si}} = \frac{1}{2}\left[\sum_{i}^{N} \Delta U\left(r_i^{n+1}\right) - \sum_{i}^{N} \Delta U\left(r_i^{n}\right)\right]$$

Contribute both kink nucleation and migration

□ Distribution of ΔU



Solute effect on kink migration process

$$\Delta E_{\mathrm{km}} = \sum_{i}^{N} \Delta G_{\mathrm{km}}^{0}(r_i^n) \quad \Delta G_{\mathrm{km}}^{0}(r) = \begin{cases} \Delta G_{\mathrm{km}}^{1\mathrm{Sol}} & r \le r_c \\ 0 & r > r_c \end{cases}$$

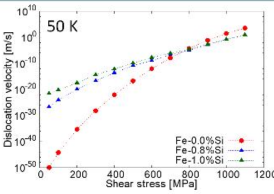
r_c : dislocation core radius

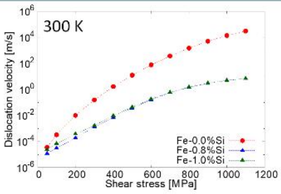
Activation energy on dislocation motion with solute effect

$$\Delta G_{\mathrm{kn}}^{+} = \left(\Delta G_{\mathrm{kn}}^{0} + \Delta E_{\mathrm{Si}}^{+}\right)\left[1 - \left(\frac{\tau}{\tau_{\mathrm{kn}}}\right)^{p}\right]^{q} \qquad \Delta G_{\mathrm{kn}}^{-} = \left(\Delta G_{\mathrm{kn}}^{0} + \Delta E_{\mathrm{Si}}^{-}\right)\left\{2 - \left[1 - \left(\frac{\tau}{\tau_{\mathrm{kn}}}\right)^{p}\right]^{q}\right\}$$

$$\Delta G_{\mathrm{km}}^{+} = \Delta E_{\mathrm{km}} + \Delta E_{\mathrm{Si}}^{+} - W \qquad \Delta G_{\mathrm{km}}^{-} = \Delta E_{\mathrm{km}} + \Delta E_{\mathrm{Si}}^{-} + W \qquad W = 0.94 b^2 w \tau$$

Solute effect on dislocation velocity





In low stress range, dislocation velocity in Fe-Si alloy is higher than that in pure iron at low temperature, although dislocation velocity in Fe-Si alloy is lower than that in pure iron at high temperature.

Solute effect on mechanical strength

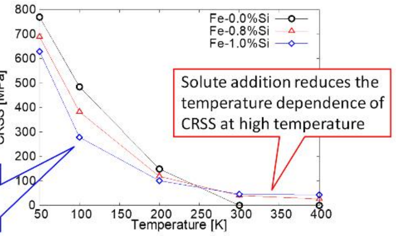
Critical resolved shear stress(CRSS) is determined as τ^* which satisfies Orowan's equation $\dot{\varepsilon}^{\mathrm{ext}} = \rho_{\mathrm{m}} b v(\tau^*)$

Estimation condition

$\dot{\varepsilon}^{\mathrm{ext}} = 1.0 \times 10^{-4}\ \mathrm{s}^{-1}$

$\rho_{\mathrm{m}} = 10^{12}\ \mathrm{m}^{-2}$

$b = 0.247\ \mathrm{nm}$



Solute addition decreases CRSS at low temperature with increasing its composition

Solute addition reduces the temperature dependence of CRSS at high temperature

想定する分野・用途

構造材料（合金）の機械的特性の制御や予測

最終目標

様々な合金に対するハミルトニアンからの強度予測結果を用いることで実現する、機械学習を用いた合金強度設計

産業界への期待・要望

マルチスケールモデリングが高度化し、その有用性が近年高まってきており、材料開発に積極的に用いてほしい